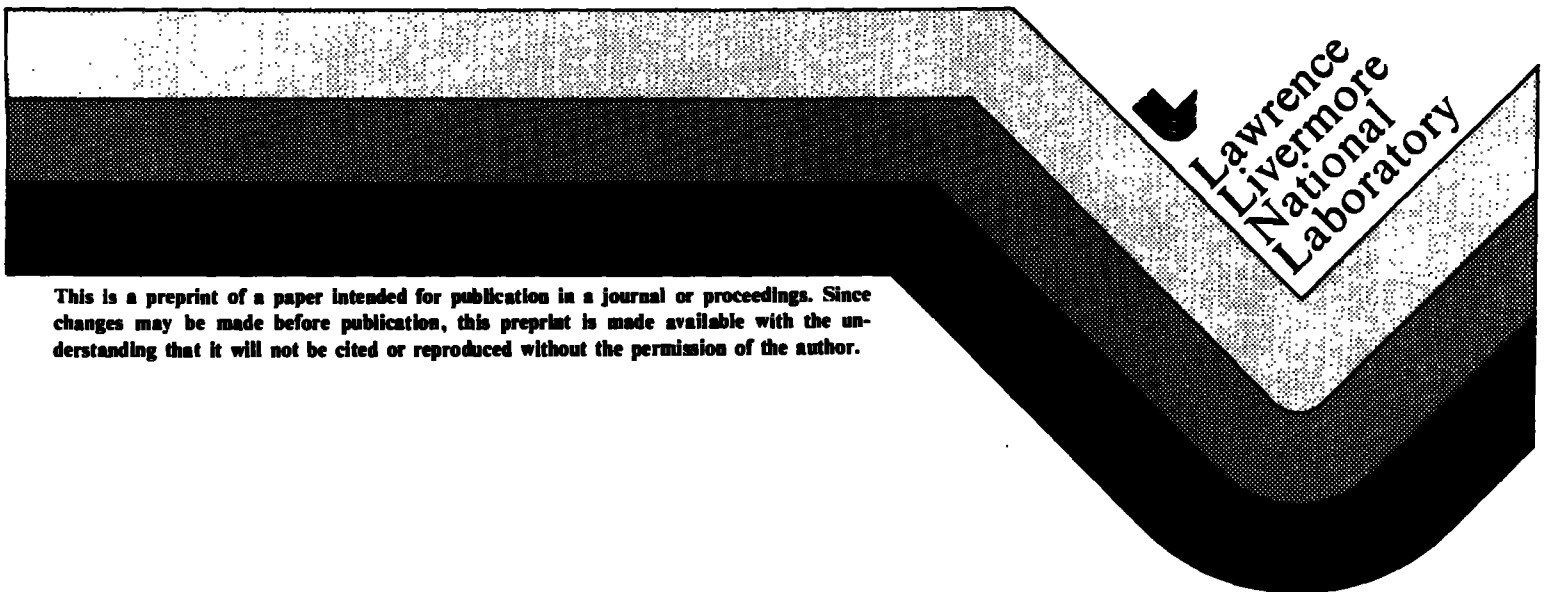# A METHOD-OF-LINE APPROACH TO SOLUTION OF PACKED-BED FLOW PROBLEMS RELATED TO UNDERGROUND COAL GASIFICATION PROCESSES

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DISCLAIMER

A METHOD-OF-LINE APPROACH TO SOLUTION OF PACKED-BED FLOW PROBLEMS RELATED TO UNDERGROUND COAL GASIFICATION PROCESSES

by

C. B. Thorsness [1]
S.-W. Kang [1]

ABSTRACT

A theoretical modeling analysis employing the method-of-line (MOL) technique is presented for characterizing reacting flows through packed beds. These flows are related to the underground coal gasification conditions in terms of combustion and multi-component chemical reactions that take place inside charring coal beds. Time-dependent, two-dimensional partial differential equations (PDE's) describing conservation of the mass, the species, the momentum, and the thermal energy are formulated. These PDE's are then recast into a set of ordinary differential equations (ODE's) with time as independent variable. The resulting ODE's are solved by applying an MOL technique developed at LLNL to multi-component flows through packed char beds. The temperature distributions near the side walls and the heat-transfer characteristics are of special interest for their implications on the cavity-wall growth behavior during UCG processes. Preliminary indications are that the MOL approach will be useful for modeling the physics of the transient, two-dimensional packed-bed flows related to the underground coal gasification conditions.

INTRODUCTION

During underground coal gasification (UCG) a considerable proportion of the process takes place in what can best be described as a packed bed. The packed bed system is a two-phase system in which gas flows past solid particles and interacts with these particles. Reactants in the gas phase move to the particle surfaces and react with them and products move back into the gas stream. In addition the possibility of strictly gas phase reactions exists when combustible gas comes in contact with injected oxygen. Also the movement of heat energy within the bed occurs from hotter zones to cooler ones (e.g. from combustion zones to wall areas). To understand the UCG process the physics of this packed bed geometry must be understood well enough to know how important process parameters, such as gas composition and coal consumption, are influenced by changes which occur in this portion of the underground system.

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In this paper we describe our recent work in developing a tool to help us understand the dynamics of the packed bed system. The aim of this work is to develop a mathematical model of the packed bed geometry embodied in a numerical computer code. The mathematical model is to be based on a reasonably fundamental description of the processes occurring including the ability to handle the movement of the solid phase. Since some of the phenomena of interest are inherently at least two-dimensional in nature the model must be able to deal with both one and two dimensional systems.

Beyond the basic desire to obtain a better understanding of the UCG process the current work is motivated by a number of more concrete goals. We want to develop a single model which would allow us to handle the various time scales associated with several important phenomena including ignition, changes in injection composition, tracer injection, and burnout of the bed. Much past work has focused on models tailored to address specific issues and as a consequence made simplifying assumptions which would not let this variety of questions to be addressed. This is not to say that models tailored to specific issues are not valuable. They are, since they often employ very economic solution schemes not available to more fundamental models. Still the advantage of development of a single model to answer a variety of questions at the expense of computational simplicity is attractive.

We also want the model to serve as a test bed for the development of simplifying assumptions used by more comprehensive models. Because of the complexity of the full range of processes encountered during UCG no truly comprehensive model of the process will be able to be based directly on the fundamental physics of the process and must instead rely on simplified descriptions of the system. The more well founded are these simplified models the better the comprehensive model. We hope the current development can lead to a tool useful in verifying and generating simplified models related to the packed portion of the UCG system.

In addition we want to explore the current computational limits imposed by computer time and memory constraints on problems related to the UCG process. Since we are mainly interested in the problem of physics and not the numerics this exploration is and will not be comprehensive. It is limited to the the use of straightforward methods of dealing with the partial differential equations which are the mathematical statement of the model.

Finally we want a model which can help us explore the wall growth problem and be useful in a detailed analysis of data that we hope will be forth coming from our proposed large laboratory scale experiments. The wall growth question is one of determining the controlling parameters for the incorporation of virgin coal in the wall into the rubble bed of the cavity. This involves, among other things, questions of heat and mass transport to the wall region which a packed bed model could help address. The wall growth phenomenon is one of the several phenomena we would like to address in a series of large laboratory experiments (one-fifth field scale), in which we hope to obtain enough detailed information to warrant the use of a relatively detailed description of the packed bed portion of the system to analyze the results.

Even though a considerable amount of work has been done in the past on modeling gasification of coal in packed beds we were not able to find a completed effort which would serve as a suitable starting point for the current work. Past work on UCG packed bed models, (Gunn and Whitman 1976) and (Thorsness et al 1978), are of limited usefulness because there is no

straightforward method of extending them to more than one dimension and including all the time dependent phenomena. In the surface gasification literature at least one nominally two dimensional model is described (Denn et al 1982), however the model was primarily developed to analyze steady-state operation and in addition the system considered is such that two dimensional gas flow is not considered. We have adopted from this latter work, however, the basic scheme of dealing with the heterogeneous gas solid reactions.

In selecting a method to solve the mathematical system of equations representing the model we have adhered to the following basic guidelines. First, the method chosen must be applicable, at least in theory, to one, two and three dimensional geometries. Second, the method must be suitably general and suitably stable to allow the physics of the model to be changed without requiring the basic solution scheme to be changed. Finally, the method must be embodied in currently available software. Based on these considerations the solution method chosen involves the spatial discretization of the governing partial differential equations coupled with a suitable ordinary differential equation solver to deal with the time dimension. This is the Method of Lines. The ordinary differential equation solver must be one able to handle the stiff-equation sets resulting from the nature of the problem and the spatial discretization. We have chosen to use the method of Gear (1971) which has been used in the past to develop some general purpose one dimensional partial differential equation solvers (Sincovec and Madsen 1975). This method is embodied by the routine LSODE developed by Alan Hindmarsh (1980) at LLNL .

Finite difference techniques have been used to develop the spatially discretized equations. Upwind or donor cell differencing of the convective terms has been employed to deal with spatial "wiggles" in convected quantities which can occur in certain areas of the system. The choice of the finite difference approach as a starting point was made primarily because of the authors' familiarity with this method. We feel that a finite element method will be more appropriate in handling the curved boundary problems of interest and have taken an initial look at both orthogonal collocation on finite elements and the Galerkin finite element method. We were initially drawn to the collocation method because of its successful use on a surface gasifier problem (Denn et al 1982). But after some preliminary testing we now feel that the Galerkin method is probably more suitable.

BASIC MODEL EQUATIONS

The basic conservation equations used in the model are mass and energy balance equations on the solid and gas phases. The gas phase mass balance equations are:

overall gas conservation

$$\frac{\partial(\epsilon C)}{\partial t} = -\bar{\nabla}\cdot(C\bar{v}) + \sum_{i=1}^{n} s_i \qquad (1)$$

gas species conservation

$$\frac{\partial(\epsilon c_i)}{\partial t} = -\bar{\nabla}\cdot(c_i\bar{v}) + \bar{\nabla}\cdot(DC\cdot\bar{\nabla}y_i) \qquad (2)$$
$$+ s_i$$

A definition of all variables is given at the end of the paper in the nomenclature section.

The solid phase mass balances are:

overall solid conservation

$$\frac{\partial[(1-\epsilon)\rho_s]}{\partial t} = -\bar{\nabla}\cdot(\rho_s\bar{v}_s) + \sum_{k=1}^{m} s_k^* \qquad (3)$$

solid species conservation

$$\frac{\partial[(1-\epsilon)w_k\rho_s]}{\partial t} = -\bar{\nabla}\cdot(w_k\rho_s\bar{v}_s) + s_k^* \qquad (4)$$

The overall phase conservation balances appear to be redundant since the sum of the species conservation equations is the overall conservation equation. They are included here however because they are used in the current implementation to develop equations which allow the gas and solid phase velocities to be calculated.

The energy balance for the entire system assumes that gas and solid temperatures are equal at a given point in space. The energy balance is given by the following equation

$$\frac{\partial}{\partial t}\left[\epsilon\sum_{i=1}^{n}(c_ih_i) + (1-\epsilon)\rho_s\sum_{i=1}^{m}(w_ih_i^*)\right] \qquad (5)$$

$$= -\bar{\nabla}\cdot\left[\sum_{i=1}^{m}(\bar{j}_ih_i)\right] - \bar{\nabla}\cdot\left[\bar{v}_s\rho_s\sum_{i=1}^{m}(w_ih_i^*)\right]$$

$$+ \bar{\nabla}\cdot(k\bar{\nabla}T)$$

where $\bar{j}_i = \bar{v}c_i - DC\bar{\nabla}y_i$

CURRENT IMPLEMENTATION

The initial model, described here, is a compromise between completeness and expediency. We wanted enough complexity so that an evaluation could be made of the utility of the

current approach yet we did not want to spend an undue amount of time developing detailed model physics. The current model employs only two solid species (ash and carbon) and six gas species (nitrogen, oxygen, hydrogen, carbon monoxide, carbon dioxide and water vapor). The extension to more gas species is trivial, only requiring a definition of reaction kinetics for the component, while the extension to more solid species would be slightly more involved. One or rectangular two dimensional problems can be investigated with the current model.

The overall mass balance equations for both the gas and solid phases are not used directly but are instead expanded to obtain equations from which gas and solid velocities can be calculated. Currently only very crude models are employed. In the gas phase we assume Darcy's law holds. This means that velocity and pressure in the bed are related by

$$\bar{v} = -\frac{\Gamma}{\mu}\bar{\nabla}P \qquad (6)$$

Using this relation and assuming the ideal gas law holds one can view equation (1) as an equation for system pressure from which gas velocities can be calculated. In the actual solution scheme however, the equation is written as an equation for overall concentration to preserve the conservative nature of the equation.

In the solid phase we allow one of three assumptions to be made. The first is that the solids do not move at all. In this case equation (3) for the overall solid is not required and is not used. In the second assumption the solid velocity is simply set at a constant value in the vertical direction and zero in the horizontal direction. The final option is a first attempt at a simple model of bed settling model. Here we assume that the overall bed density remains

constant and solids only move in a straight downward direction. This removes the time rate of change term from equation (3) and allows it to be integrated in the vertical space direction to give the solid velocity as a function of position at any time

$$v_s = v_{s_o} + \frac{1}{w_c \rho_s} \int_0^y s_c^* dy \qquad (7)$$

For simplicity we assume that most of the solid and gas properties are not functions of pressure, temperature or composition. The relaxation of this constraint within the framework of the current model would be straightforward.

Of the physical models employed the kinetic model is the most elaborate. It represents an extension of the models employed by Yoon et al (1978). Two basic kinetic models for the heterogeneous reactions representing the extremes of behavior have been used. Both are based on the idea of a single initial particle size, but extension to a distribution of initial sizes is possible. The models consider that the apparent rate of an individual reaction may be controlled by gas film diffusion external to the particle, by diffusion through an ash layer, by diffusion into the reacting particle, or by intrinsic surface reaction rate.

In the first of the two models, the shell progressive (SP) model it is assumed that a core of unreacted solid is surrounded by a shell of ash. For the gas phase reactants to reach the unreacted core they must not only diffuse through the external gas film but also through this ash layer. In the second model, the ash segregation (AS) model, it is assumed that the ash falls away from the particle leaving unreacted material exposed to the gas stream.

The model considers three reactions that follow these heterogeneous reaction models:

$$C + 1/2\ O_2 \rightarrow \alpha\ CO + (1-\alpha)\ CO_2$$

$$C + CO_2 \leftrightarrow 2\ CO$$

$$C + H_2O \leftrightarrow CO + H_2$$
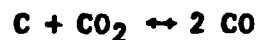
No carbon hydrogen reaction is included since methane is not considered in current set of allowed gases. The rate of reaction for the SP model for these reactions is given by

$$r = \frac{\pi N\ (c - c_{eq})}{\dfrac{1}{k_c d_p^2} + \dfrac{(1-F)}{2D_e d_p} + \dfrac{6}{n k_r \rho_c d_u^3}} \qquad (8)$$

With the AS model no ash layer is present and the reaction rate is given by

$$r = \frac{\pi N\ (c - c_{eq})}{\dfrac{1}{k_c d_p^2} + \dfrac{6}{n k_r \rho_c d_p^3}} \qquad (9)$$

The particle sizes used in the correlations are assumed to be a function of position in the bed and amount of reaction which has occurred. Therefore at any one time there is a distribution of particle sizes in the bed. In the SP model the minimum particle size is function of initial particle size and ash concentration. In the AS model the unreacted solid minimum diameter is zero and there is assumed to be ash particle present having a particle diameter equal to some selected fraction of the initial particle size. Relations for particle size and other derived quantities used in the rate expressions are given in Appendix I.

In addition to the above heterogeneous reactions we add the water-gas-shift reaction

$$CO + H_2O \leftrightarrow CO_2 + H_2$$
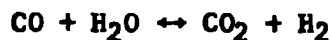
Even though it involves only gas phase species it is highly catalyzed by solid surfaces and as a result in a packed bed situation nearly all the reaction occurs on surfaces. The same basic expressions as those given above are used except that in the SP model the particles are considered uniformly active calalyst and therefore no unreacted core is considered and the rate is given by the AS model expression with appropriate particle diameters. In the AS model the overall rate is considered to be the sum of two rates, one using the unreacted particle parameters in the AS expression and one using the ash particle parameters.

In both AS and SP models it has been assumed that the intrinsic reaction rate of carbon and gas can adequately be represented by the simple expression

$$r^* = k_r \ (c - c_{eq}) \qquad (10a)$$

$$k_r = A \ exp \ (-E/RT) \qquad (10b)$$

The primary gas phase reacted is included here in a simple first order manner. The expression for the intrinsic rate of the water-gas-shift is slightly more complicated. It is taken from Govind and Shah (1984)

$$r_4^* = 568 \ RT \left(0.5 - \frac{P}{2.53 \times 10^7}\right)\left([CO] - (CO]_{eq}\right)$$

$$exp \ (-13971/T) \qquad (11)$$

The k_r used in this case in the overall rate expression includes everything except the carbon monoxide concentration.

A final strictly gas phase reaction is considered in the model. This reaction is included to allow gas phase combustion to occur. The

reaction selected was that of carbon monoxide combustion given by the following expression taken from Field et al (1967).

$$r_5 = 4.75 \times 10^5 \ [CO] \ [H_2O] \left\{ \frac{17.5 \ \frac{[O_2]}{C}}{1 + 24.7 \ \frac{[O_2]}{C}} \right\}$$

$$exp \ (-8050/T) \qquad (12)$$

Even though only carbon monoxide combustion is included the presence of the water-gas-shift allows hydrogen to be in effect also consumed by oxygen in the gas phase.

We now present some typical behavior related to the rate expressions described above. These results are for the particular conditions of ρ_B = 1000 kg/m^3, ϕ = 0.5, f= 0.25, d_0=0.025 m, g= 1.0 mol/m^2-s, a = 1.0, and constant bed-density. Figure 1 shows the effect of temperature on various reaction rates used for F=1 (full char, no ash) for which case the rates are the same for both SP and AS models. At low temperature the magnitudes of the rates are dominated by kinetics only (reaction limited)
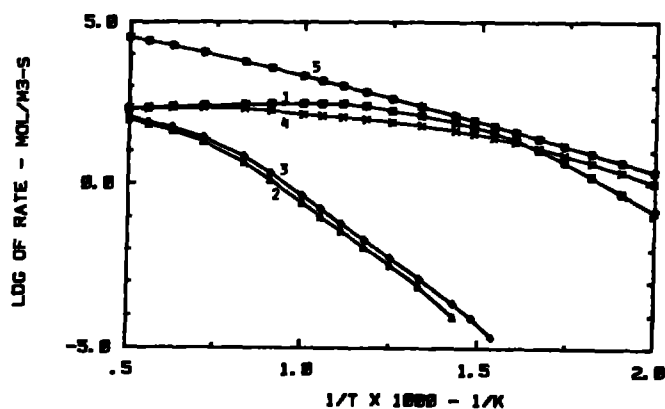

Figure 1. Reaction Rates in Packed Beds for SP and AS Models (Reaction 1: $C+O_2 \rightarrow CO+CO_2$; 2: $C+CO_2 \leftrightarrow 2 \ CO$; 3: $C+H_2O \leftrightarrow CO+H_2$; 4: $CO+H_2O \leftrightarrow CO_2+H_2$; 5: $CO+O_2 \leftrightarrow CO_2$; d_p=0.025m; g=1.0 mol/m^2-s).

and display sharp decrease with
decrease in temperature. On the other
hand at high temperatures the rates
become dominated by internal particle
diffusion and finally by external mass
flux transported to the particle
surface. This general behavior
applies to all reactions shown in
Figure 1, except for the CO + O_2
reaction. This particular reaction
takes place in gas phase under present
conditions and consequently is not
affected by mass transfer
considerations.

As the packed-bed reactions proceed,
the fraction of carbon decreases,
causing the particle sizes to become
smaller and the particle number
densities (number of particles per
cubic meters) to increase. The
quantitative variations of these
properties are also given in
mathematical form in Eqs. (A.1)
through (A.14) in the Appendix. Here
we show these in graphic form (Figures
2 and 3) for both SP and AS models.
It can be seen from the figures that
the particle diameter decreases only
slightly and reaches a finite value as
the fraction of carbon reaches zero
for the SP model, whereas for the AS
model the particle size steadily
decreases and ultimately goes to zero,
consistent with the model assumed. For
the AS model ash particles are
generated as the carbon particles
undergo various reactions in the bed.
The size of the ash particles is
assumed fixed at 25 % of the initial
size, i.e., f = 0.25, and thus is
0.00625 m (see Figure 2). As particle
sizes diminish with decrease in the
carbon fraction in the bed, the number
of these carbon particles per unit
volume (number density) increases, to
satisfy the mass-conservation
condition. This is shown in Figure 3,
where the number density for unreacted
carbon particle (N) is the same for
both models and the ash particle
number density increases dramatically
as its size approaches zero. The
mathematical description of this
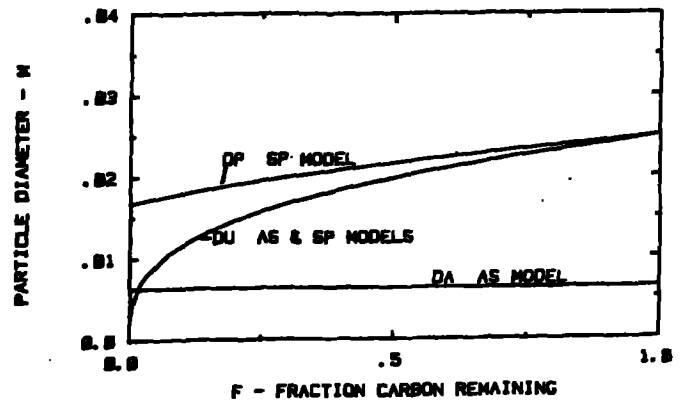behavior is given in Eqs. (A.13) and
(A.14).

Figure 2. Particle Size Changes for
SP and AS Models (Assuming Constant Bed-
Density).
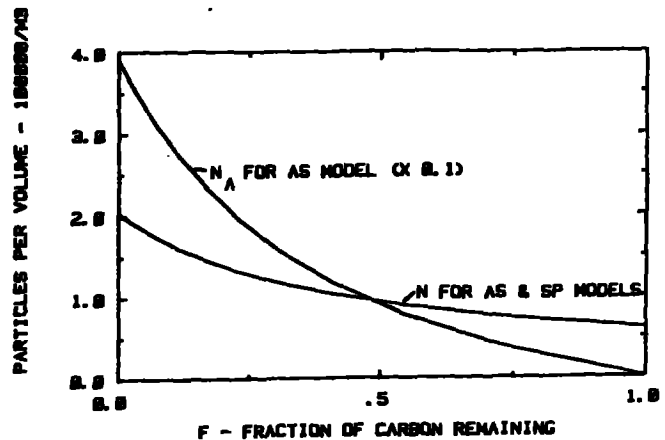
Figure 3. Particle Number-Density
Changes for SP and AS Models (Assuming
Constant Bed-Density).

The choice of either SP or AS model
determines the reaction patterns
taking place inside a packed bed as
the fraction of carbon diminishes.
Figure 4 shows that the carbon
oxidation rates decreases sharply with
decreasing carbon fraction for SP
model, while those for AS model
change only slightly for a sizeable
range of carbon fraction and even
displays a moderate increase before
finally going to zero. This difference
in rates is a result of the difference
in disposition of the ash in the two
models. In the AS model the ash falls
away leaving the surface directly
accessable to the gas phase, while in the
SP the ash adheres to the char surface

Figure 4. Effect of SP and AS Models on Carbon-Oxidation Rates.

and therefore limits access of the oxygen to the carbon surface.

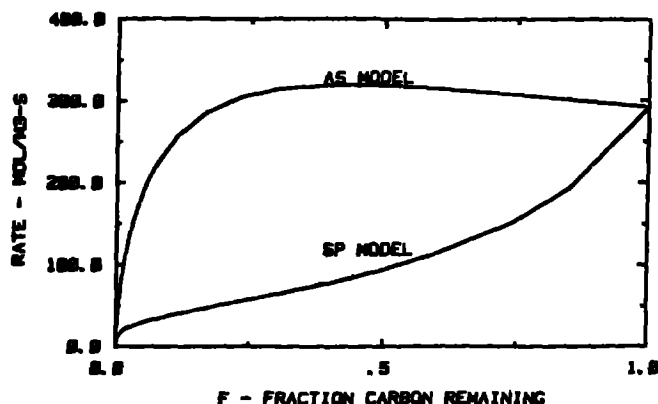The rates for the water-gas-shift reaction are given in Figure 5 as a function of carbon fraction for both SP and AS models. Only moderate change is seen for the SP model, in contrast to that for the AS model. Such difference in sensitivity between the two models is caused by the difference in available surface areas acting as catalyst for the WGS reaction. We note in passing that only pure (intrinsic) kinetic reactions prevail for the reactions involving carbon with CO_2 and H_2O (Reactions 2 and 3 in Figure 1), and thus these reactions produce the same rates for both models.
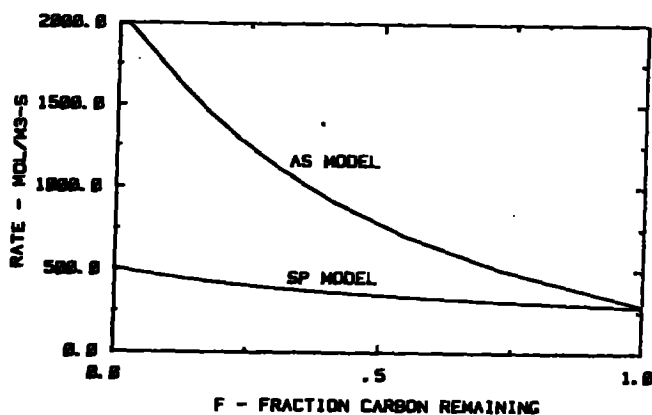

Figure 5. Effect of SP and AS Models on Water-Gas-Shift Rates.

Consideration of both AS and SP models for the present problem is useful because these two models should represent extremes in possible behavior. This fact then enables us to bracket the magnitudes of these relevant reactions taking place in the bed.

DISCUSSION

A number of test problems have been run with the model. For the most part we have found the solution scheme (i.e. LSODE) to be very robust. The highly nonlinear nature of the problem, the variation of many orders of magnitude in rate constants, and the essential water-gas-shift equilibrium existing at many locations in the system have all seemed to be handled adequately. The only limitation we have imposed on the problem physics for the sake of easing the computational burden has been the limitation of the gas phase oxidation reaction to rates reached at 900 K. At this temperature the rate is much faster than any other reaction at any temperature and thus its limitation probably leads to no significant change in the evolution of the system.

In the following we first describe the computational limits placed on the model by computer resource considerations and then give several sample calculations performed in both one and two dimensions.

Computer Resource Limitations

The model has been run on both a CDC-7600 computer and a CRAY-1 computer. In the following the the computational times and memory limits will be those for the CRAY-1 except where noted. The equivalent 7600 computational times can be obtained from the CRAY times by multiplying by a factor of three.

For one-dimensional problem the computer limitations are modest. The

amount of computer storage required is given approximately by the formula

$$\text{floating point words} \cong 6\, n_y\, (3+n)^2 \quad (13)$$

Where n_y is the number of nodes used in the discretization and n is the number of gas species. The number of dependent variable is (3+n) since three equations are required to handle the system pressure, the system temperature and the solid carbon species balance. With n equal to six the number of nodes which can be used on the two million word CRAY is about 4000. This is far more than one would ever need. In practice the number of nodes required is dictated by two primary factors, the size of the physical system being modeled and the accuracy required. Since upwind differencing has been used the constraint of spatial wiggles in convected quantities is eliminated, however the concern for the relative importance of numerical dispersion in the problem needs to be considered. In the test runs done to date we have found the most severe limit is imposed by the sharp nature of particle size transition region. Large node spacing leads to periodic changes in computed quantities driven by the periodic variation in average particle size near the combustion front. Depending on the question being investigated the magnitude of these variations which can be tolerated changes. We have found for a bed one meter long composed initially of 2.5 cm. particles about 41 equally spaced nodes are required to reduce the periodic changes to relatively small levels. However if average gas composition is the desired result 21 and even 11 node systems yield the same results. The sharpness of the particle size transition is accentuated by the crude solid motion model used. One would expect that dispersive effects in the settling process would tend to smear this transition and lessen the resolution needed by the model.

The computer time required for the 41 node one-dimensional problem to a point where all the carbon originally in the bed is consumed is 2.3 minutes. About 7 minutes is required to turn the entire bed to ash (note, carbon is fed into the bed to maintain constant density in the case run.) Preliminary results indicate that for a given physical system the computation time to reach a specified problem time is proportional to the number of equations (number of nodes times number of dependent variables) raised to the 1.5 power. Consequently one-dimensional problems involving 200 nodes and 7 or 8 gas species would seem feasible. The computer code representing the solution of the model equations allows parameters to be changed during runs and allows repeated restarts of a given problem from a selected time. This feature can greatly reduce the time required in systematic studies and as a result would allow even larger systems to be investigated.

Two-dimensional problems run into much more severe computer limitations. The memory required for a two dimensional problem is given approximately by

$$\text{floating point words} \cong 3\, n_y\, n_x^2\, (3+n)^2$$

$$(14)$$

This means to maintain the problem entirely within the memory of a two million work CRAY machine the maximum problem size would be on the order of $n_y=32$ and $n_x=16$. The use of virtual memory could extend this size but the computational time would be prohibitive. The largest test case we have run is a 11 by 8 node system representing a 1 meter by 1 meter bed. This problem took 25 minutes of computer time to burn up all the carbon originally within the bed and 45 to 60 minutes, depending on the exact problem, to turn the bed completely to ash. The computation time appears to scale like $(n_y \times n_x^2)^{1.5}$. The computation time

appears to be a more severe limit than the size limit. It is our feeling that computer resources impose a significant limitation on two-dimensional problems requiring runs covering the entire evolution of a bed. However, for problems requiring shorter intervals the computational time may be acceptable.

The results on computational effort for the one and two-dimensional problems indicate that most computations related to truly three-dimensional problems would not be feasible. Three dimensional problems which are axisymmetric, however fall under the same constraints as the two dimensional problems discussed above. Also three dimensional problems in which only very short time periods are of interest could be approached. We have no current plans to extend the model to a true three-dimensional geometry.

Sample Computations

In the sample calculations described below the value of model parameters given in Table 1 were used. The geometries used were that of a bed 1 meter long bed for the one-dimensional runs and a bed 1 meter by 1 meter for the two-dimensional calculations. In the two-dimensional runs injection gas was input to the center and bottom of the bed allowing symmetry to reduce the required computations to one half of the bed. In both cases a constant density bed was assumed with solids being fed in at the top of the bed to maintain the prescribed one meter height. Also in all cases the SP kinetic model was employed for the heterogeneous reactions.

The one-dimensional sample calculations were run using an equally spaced 41, 21 and 11 node system with a steam/oxygen injection rate of 1 mol/s/m^2 and an initial steam/oxygen mole ratio of 3/1. To initiate the burn a small zone, 1.5 cm. long, was set at 750 K. Similar produced gas composition results were obtained in

Table 1. Parameters used in sample calculations.

α	1.0	
c_g	47.0	J/mol-K
D_m	5.5×10^{-4}	m^2/s
D	3.2×10^{-3}	m^2/s
c_s	1500.	J/kg-K
w_{c0}	0.7	
k	1.2	w/m-K
f	0.25	
ϵ	0.5	
θ	0.3	
ρ_s	1000	kg/m^3
Γ/μ	1.0×10^{-6}	m^2/Pa-s
T (injected gas)	350.	K
P (at exit)	1.0×10^{5}	Pa
T (initial)	350.	K
T (of input solid)	350.	K
d_0	0.025	m

Kinetic parameters	A (1/s)	E (kJ/mol)
$C + O_2$	17.7	112.
$C + CO_2$	0.0024	145.
$C + H_2O$	0.0041	145.

all runs. However, as the number of nodes decreases the magnitude of periodic changes in the system related to the sharp nature of the particle size changes increases and are quite large for the 11 node system. In Figs. 6 and 7 exit gas composition and temperature are shown for the 41 node run over the ignition phase of the burn. This phase actually includes a number of changes. The first, resolved by the model solution but not apparent on the figures, is the pressuring up of the system and the sweeping out of gas initially in the bed. This happens during the first minute. The second change (just visible in the plots) is the complete

disappearance of oxygen as the ignition region begins to heat up. This occurs in the first 5 minutes. Over the next 30 minutes the ignition region heats up sufficiently so that significant gasification is occurring. This is indicted in the Figure 6 by the rapid change in non-oxygen gas species concentration. The final transition which can be associated with start-up occurs from the 2 1/2 to 3 hour time interval in which the top of the bed is finally heated. Gas composition changes slightly during this transition since no longer is a thermal front associated with heating of initially cold solid present in the bed.
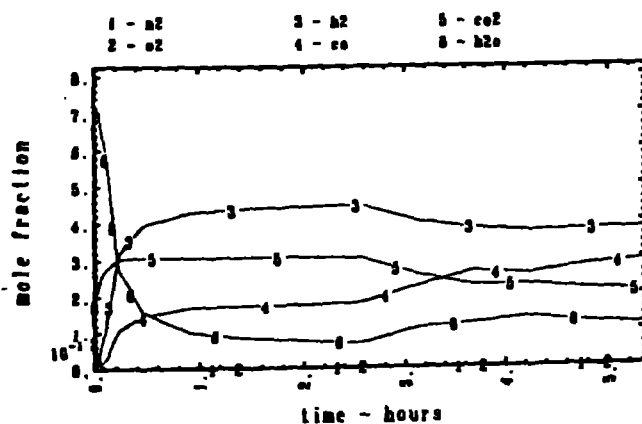
Figure 8 shows the exit gas composition for the same run over the period of 40 hours during which the bed is completely turned to ash. Four transitions are illustrated. The first is the ignition phase occurring over the first 3 to four hours. At hour 10 the injection gas was changed from a 3/1 steam/oxygen ratio to a 4/1 ratio. Then at hour 20 the ratio is changed to 1/1. Transition to new exit gas concentrations takes about 1 hour for the 3/1 to 4/1 transition and about 2 hours for the 4/1 to 1/1 transition. The final change occurring from hour 27 to 33 is the final consumption of the carbon remaining in the bed. The periodic changes in the gas composition described above are visible. Notice for the 1/1 period they essentially disappear, since temperatures are very hot and details near the burn front where the sharp particle size transition occurs are totally masked by downstream reactions.

Figure 6. Exit Gas Composition for the Ignition Period of the 1-D Sample Run.
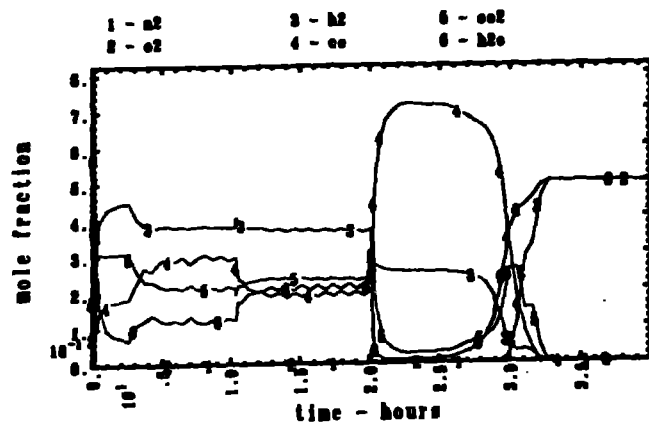
Figure 8. Exit gas composition for the 1-D sample run from ignition to complete consumption of carbon in the bed.

Figure 7. Exit Gas Temperature for the Ignition Period of the 1-D Sample Run.

As a test of the models ability to handle the two-dimensional (2-D) geometry several sample runs were done for the 1 meter by 1 meter system mentioned above. In these runs steam/oxygen at a 3/1 mole ratio was injected at a rate so that the

effective feed to the bed was one mole/s/m^2. In Table 2 exit gas composition after ten hours for two different 2-D runs as well as results from an equivalent 1-D run are given. The 2-D runs were the same except for the boundary condition imposed at the side wall. In one case the wall was assumed to be an insulated impermeable boundary and in the other case the boundary condition simulating the in flow of gas from a coal face was used. In this latter case the influx wall gases were assumed to be 9 (mole) % nitrogen (used as a tracer), 31% hydrogen, 7% carbon monoxide, 5% carbon dioxide and the remainder steam. The correlation relating heat flow to the wall and gas evolution at the wall was chosen so that gas would begin to evolve at a wall temperature of 800 K and increase linearly with temperature so that at 810 K gas evolution equivalent to a wall regression rate of 1 meter/day would be established. The base state of the the influxing gas is 298 K with the water as liquid. This means that the heat load is roughly equivalent to that needed to dry and pyrolyze an amount of coal which would yield the influx gas. This formulation has the effect of essentially locking the wall region to a temperature near 800 K and allowing the computed wall temperatures to be equated to local equivalent wall regr.ssion rates. Table 2 shows that at the ten hour

point the 1-D and the insulated 2-D systems yield similar exit gas concentrations as one would expect, however the difference in steam content is probably significant and related to somewhat different effective gas residence times in the two systems. The gas composition for the wall gas flux case has a significantly lower carbon monoxide level resulting from the cooling effect of the wall and the steam content is higher due to the high steam content of the influxing gas.

Some further results from the gas influx run are shown in Figure 9, showing the distribution of ash and char at two different times along with the amount of heat transfer to the wall represented as an equivalent wall regression rate. The 10.15 hour configuration represents a case where the oxygen has not reached the region of wall. The equivalent wall regression rate decreases from bottom to top primarily reflecting the relative proximity of the burn front. At 40.15 hours the system has evolved into one where nearly all the char in the bed has been consumed and the burn front is near the wall. In this case the equivalent wall rate is about twice as large, on the average, as in the earlier case. It is clear the evolution of the bed shown here is artificial in that no actual movement of the wall is occurring. In the

Table 2. Exit gas composition from three different test runs at 10 hours.

Gas component	Exit gas composition in mole percent		
	1-D run	2-D insulated wall	2-D gas flux at wall
Hydrogen	38	36	37
Carbon monoxide	29	27	20
Carbon dioxide	21	22	·23
Water vapor	12	16	19
			(Average wall gas flux equivalent to wall rate of 0.2 m/day)

future we are going to consider the possible inclusion of wall motion; however, we feel the current implementation is useful in that various assumed bed configurations can be run to determine what wall regression rates would be present and whether these rates are consistent with the assumed geometry.
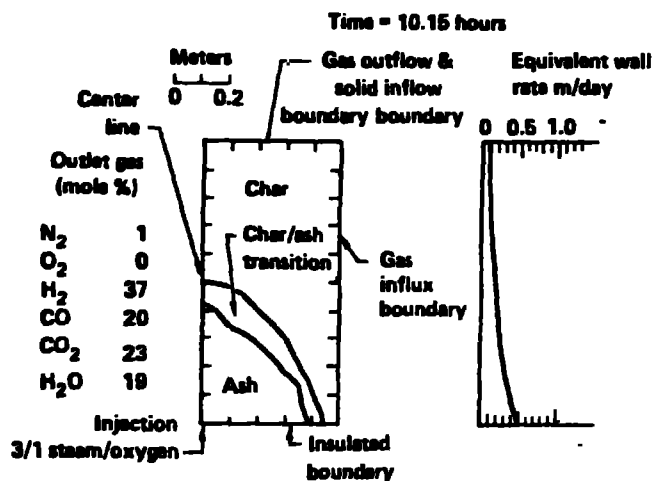

Figure 9a. Results from the 2-D sample run in which the gas enters at the side wall in proportion to heat flux to the wall. Time=10.15 hrs.
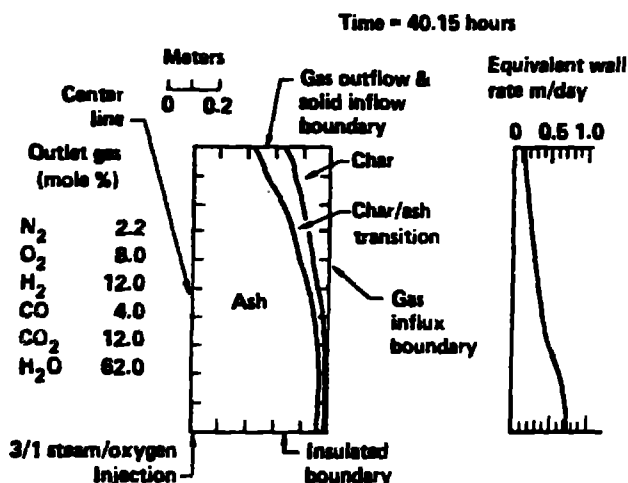

Figure 9b. Results from the 2-D sample run in which the gas enters at the side wall in proportion to heat flux to the wall. Time=40.15 hrs.

FUTURE PLANS

Based on the calculations we have done so far the use of the model to look at one-dimensional geometry questions and two-dimensional problems where the prime interest is in performance in a given configuration, and not long term system evolution, appears completely feasible. With this in mind the focus of our effort will be on the following:

* Addition of other reactions and species to the model (e.g., methane).

* Comparison of calculations to surface gasification models and data.

* Utilization of the model to evaluate and extend simple relations used in other models (e.g., CAVSM) (Thorsness et al 1983).

* Possible use of finite element formulations to allow curved or irregular 2-D systems to be better approximated.

Incorporation of a wall movement algorithm may be considered. If included it would require that long duration 2-D problems be run. Before undertaking such an extension more consideration of the ultimate computer resource limitations will be necessary. This includes the evaluation of other solution schemes for the time domain and the estimation of spatial resolution limits imposed by the physics of the problems of interest.

APPENDIX. PARTICLE SIZE AND RELATED KINETIC PARAMETERS

Both the SP and AS kinetics models given in equations 8 and 9 require several parameters to be calculated. These are the various particle diameters (d_p, d_u, and d_a), the particle number densities (N and N_a), the gas film mass transfer coefficient (k_c), the effective mass diffusivity inside a particle (D_e), and the effectiveness factor (η). Different relations are used for the particle sizes and number densities depending on the kinetic and solid motion assumptions made. For all

-14-

assumptions the basic film coefficient and effectiveness factor relations are the same.

Particle size and particle number densities used in the kinetic models are given by simple relations for the case in which number density of the char particles do not change. For a zero solid velocity or constant imposed bed velocity the relations for particle size and particle number density are as follows.

SP model:

$$d_p = d_o \tag{A.1}$$

$$d_u = F^{1/3} d_o \tag{A.2}$$

$$N = \frac{6 (1-\varepsilon)}{\pi d_o^3} \tag{A.3}$$

AS model:

$$d_u = F^{1/3} d_o \tag{A.4}$$

$$d_a = f d_o \tag{A.5}$$

$$N = \frac{6 (1-\varepsilon)}{\pi d_o^3} \tag{A.6}$$

$$N_a = N \frac{w_{ao} (1-F)}{f^3} \tag{A.7}$$

The fraction of original carbon remaining (F) is obtained from local carbon and ash densities and original weight fractions of ash and carbon and bed density.

The relations for the case in which the constant bed density assumption is made are however slightly more complicated. The equations for particle size and number density for the constant bed density (and external porosity) assumption are the following.

SP model:

$$d_p = \left[(1-w_{ao}) d_u^3 + w_{ao} d_o^3 \right]^{1/3} \tag{A.8}$$

$$d_u = F^{1/3} d_o \tag{A.9}$$

$$N = \frac{6 (1-\varepsilon)}{\pi d_p^3} \tag{A.10}$$

AS model:

$$d_u = F^{1/3} d_o \tag{A.11}$$

$$d_a = f d_o \tag{A.12}$$

$$N = \frac{6 (1-\varepsilon)}{\pi d_o^3 [F + w_{ao}(1-F)]} \tag{A.13}$$

$$N_a = \frac{w_{ao}(1-F) N}{f^3} \tag{A.14}$$

The appropriate particle size is used in obtaining the external mass transfer coefficient (k_c) and the effectiveness factor (η) used in the rate expressions. The mass transfer coefficient is obtained from Sen Gupta and Theodus (1963).

$$k_c = \frac{2.06 RT}{\varepsilon P} (Sc)^{-0.092} \left(\frac{PD}{d_p gRT} \right)^{0.575} g \tag{A.15}$$

Following Yoon et al (1978) the effectiveness factor for the heterogeous reactions are defined by

$$\tau = \frac{d_p}{6} \left(\frac{k_r \rho^*}{D_e} \right)^{1/2} \tag{A.16}$$

$$\eta = \frac{1}{\tau}\left[\frac{1}{\tanh{(3\tau)}} - \frac{1}{3\tau}\right] \qquad (A.17)$$

with the effective diffusivity approximated by

$$D_e = \phi D_m \qquad (A.18)$$

For the reactions involving carbon the ρ^* is the density of carbon in the unreacted particle and the porosity ϕ used in the effective diffusivity is that of the unreacted particle. For the water-gas-shift reaction ρ^* is the total mass density of the ash or unreacted particle as appropriate and corresponding ϕ is used to obtain the effective diffusivity.

NOMENCLATURE

A	=	Pre-exponential rate constant (1/s)
C	=	Total gas concentration (mol/m^3)
c_i	=	Concentration of gas species i (mol/m^3)
c_{eq}	=	Equilibrium concentration of a gas (mol/m^3)
c_g	=	Average gas heat capacity (J/mol-K)
c_s	=	Average solid heat capacity (J/kg-K)
d	=	Diameter (m)
d_a	=	Ash particle diameter (m)
d_p	=	Particle diameter (m)
d_u	=	Unreacted particle diameter (m)
d_0	=	Initial particle diameter (m)
D	=	Effective mass dispersion in bed (m^2/s)
D_e	=	Effective gas diffusivity inside a particle (m^2/s)
D_m	=	Average molecular diffusivity (m^2/s)
E	=	Activation energy for rate constant (J/mol)
F	=	Fraction of original carbon remaining
f	=	Ash particle size fraction
g	=	Average molar gas flux (mol/m^2-s)
h_i	=	Enthalpy of gas species i (J/mol)

h_k^*	=	Enthalpy of solid species k (J/kg)
j_i	=	Total flux of gas species i (mol/m^2-s)
k	=	Effective bed thermal conductivity (W/m-K)
k_c	=	Gas film mass transfer coefficient (m^2/s)
k_r	=	Reaction rate constant (1/s)
m	=	Number of solid species
n	=	Number of gas species
n_x	=	Number of nodes in x-direction
n_y	=	Number of nodes in y-direction
N	=	Number of particles per volume of bed (1/m^3)
N_a	=	Number of ash particles per volume of bed (1/m^3)
P	=	Pressure (Pa)
r	=	Reaction rate per volume of bed (mol/m^3-s)
r^*	=	Intrinsic reaction rate (mol/m^3-s)
r_1^*	=	Intrinsic rate of reaction 1 (mol/m^3-s)
R	=	Gas constant (J/mol-K or Pa-m^3/mol-K)
s_i	=	Species i gas source per volume of bed (mol/m^3-s)
s_k^*	=	Solid species k source per volume of bed (kg/m^3-s)
s_c^*	=	Solid carbon source per volume of bed (kg/m^3-s)
Sc	=	Schmidt number
t	=	Time (s)
T	=	Temperature (K)
v	=	Superficial gas velocity (m/s)
v_s	=	Superficial solid velocity (m/s)
v_{s0}	=	Superficial solid velocity at the bottom of the bed (m/s)
w_{a0}	=	Initial weight fraction of ash in solid
w_c	=	Mass fraction carbon in solid
w_{c0}	=	Initial weight fraction of carbon in solid
w_k	=	Mass fraction of solid species k
x	=	Horizontal coordinate (m)
y	=	Vertical coordinate (m)
y_i	=	Mole fraction of species i
α	=	Fraction of combusted carbon going directly to carbon monoxide
ρ_s		Average density of solid particle (kg/m^3)
ρ_c		Carbon density in unreacted solid (kg/m^3)

ρ^* = Reactive solid density (kg/m^3)

ϵ = Bed porosity external to particles

η = Reaction effectiveness factor

Γ = Permeability (m^2)

μ = Average gas viscosity (Pa-s)

ϕ = Porosity internal to a particle

τ = Thiele modulus

Subscripts

i = Gas species: 1 - N_2; 2 - O_2; 3 - H_2
                  4 - CO; 5 - CO_2; 6 - H_2O

k = Solid species: 1 - carbon; 2 - ash

l = Reaction: 1 - $C+1/2O_2$; 2 - $C+CO_2$;
              3 - $C+H_2O$; 4 - $CO+H_2O$;
              5 - $CO+1/2O_2$

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REFERENCES

Denn, M., J. Wei, W.-C. Yu, and R. Cwiklinski. 1982. Detailed Simulation of a Moving-Bed Gasifier. *EPRI Report AP-2576.*

Field, M. A., D. W. Gill, B. B. Morgan, and P. G. W. Hawksley. 1967. Combustion of Pulverized Coal. *Cheney & Sons Ltd.* 322-325.

Gear, C. W.. 1971. The Automatic Integration of Ordinary Differential Equations. *Communication of ACM* 14, 176.

Govind, R. and J. Shah. 1984. Modeling and Simulation of an Entrained Flow Coal Gasifier. *AIChE J.* 30, 79.

Gunn, R. D. and D. L. Whitman. 1976. An In Situ Gasification Model (Forward Mode) for Feasibility Studies and Design. *Laramie Energy Research Center, Report* LERC/RI-76/2.

Hindmarsh, A. C. 1980. Two New Initial Value Ordinary Differential Equation Solvers. *ACM Newsletter,* 15, 10.

Sen Gupta, A., and G. Thodos. 1963. Direct Analogy Between Mass and Heat Transfer to Beds of Spheres. *AIChE J.,* 9, 751.

Sincovec, R. F. and N. K. Madsen, 1975. Software for Nonlinear Partial Differential Equations. *ACM Transactions on Mathematical Software* 1, 232 .

Thorsness, C. B., E. A. Grens, and A. E. Sherwood. 1978. A One-Dimensional Model for In Situ Coal Gasification. *Lawrence Livermore National Laboratory, Report UCRL-52523.*

Thorsness, C. B. and R. J. Cena. 1983. An Underground Coal Gasification Cavity Simulator with Solid Motion. *Lawrence Livermore National Laboratory, Report UCRL-89084.*

Yoon, H, J. Wei, and M. Denn. 1978. A Model for Moving Bed Gasification Reactors. *AIChE J.* 24, 885,